Efficient numerical methods for elliptic and parabolic partial differential equations

Theses of PhD Dissertation

by

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1. Introduction

The topic of this thesis is centered around the numerical treatment of partial differential equations. Linear and nonlinear, elliptic and parabolic problems are considered. The main focus is on the development of efficient solution techniques for elliptic problems using a suitable iterative method. We also pay special attention to numerical implementations and experiments.

During the numerical solution of elliptic partial differential equations we use an abstract theoretical setting, usually working in a Hilbert or Banach space framework. Our main interest lies in developing Newton-type methods and conjugate gradient methods, within a finite element framework. In general on iterative methods we refer to [Axe96, FK02].

Our investigations are twofold. Firstly, we study problems whose numerical solution is still considered as a challenge in the literature. We show robust convergence results for convection-dominated elliptic problems, in contrast to the result of Kirby [Kir10]. The numerical study of the nonlinear Schrödinger equation leads to the extension of the results of the variable preconditioning Newton-like method developed by Karátson and Faragó [KF03] to the case of complex Hilbert spaces.

Secondly, we are interested in the computational performance of numerical methods: efficiency of the presented gradient and Newton-type methods, accuracy of a sharp upper global a posteriori error estimator developed by Karátson and Korotov [KK09]. Based on our presented numerical experiments we suggest and investigate possible improvements and discuss practical aspects as well.

The thesis is based on the author's papers [AKK14, Kov12, Kov14, KK13].

2. Preliminaries

The elliptic problems treated in the thesis mostly fit into the following general class of nonlinear problems, see also [FK02, Chapter 6].

Let Ω be a sufficiently smooth d-dimensional open and bounded domain with boundary $\partial\Omega$. The boundary $\partial\Omega$ is decomposed into the Dirichlet and Neumann boundary, Γ_D and Γ_N, while ν is the outward normal.

We consider the following *nonlinear elliptic* problem with mixed boundary conditions:

$$\begin{cases} -\operatorname{div}\big(f(x,\nabla u)\big) + q(x,u) = g & \text{in} \quad \Omega, \\ u = 0 & \text{on} \quad \Gamma_D, \\ f(x,\nabla u)\cdot\nu + s(x,u) = \gamma & \text{on} \quad \Gamma_N. \end{cases} \tag{1}$$

The weak formulation is

$$\int_\Omega \Big(f(x,\nabla u)\cdot\nabla v + q(x,u)v \Big) + \int_{\Gamma_N} s(x,u)v\,\mathrm{d}\sigma = \int_\Omega gv + \int_{\Gamma_N} \gamma v\,\mathrm{d}\sigma \qquad (v \in H_D^1(\Omega)) \,, \tag{2}$$

where the Hilbert space is defined as $H_D^1(\Omega) = \big\{ u \in H^1(\Omega) \,\big|\, u|_{\Gamma_D} = 0 \big\}$, with a suitable inner product.

It is well known, [FK02, Section 6.1], that using the Riesz representation theorem the above problem can be written as the abstract problem $\langle F(u), v\rangle = \langle b, v\rangle$ in the above Hilbert space. Furthermore, it has a unique weak solution due to [FK02, Theorem 6.4]. We note that many possible generalizations can be treated similarly.

3. Convection-dominated elliptic problems: robust estimates for streamline diffusion preconditioning

Convection-dominated elliptic equations form an important class in the modelling of stationary convection–diffusion problems, and hence are the subject of intense research, with vast literature, cf. [ESW14, Kir10], and the references therein.

A common point is that standard finite element discretizations are inadequate for such problems, they require a very fine mesh, otherwise they behave poorly. Hence, the finite element method is replaced by some stabilized version, such as the so-called *streamline diffusion finite element method*, see for example [ESW14, Chapter 3].

The arising linear systems are generally solved by some preconditioned (conjugate gradient type) iterative method. The convergence of these iterations is also influenced by the convection-dominated character. To be precise, the convergence becomes slow if the coefficient ε of the diffusion term is small. To overcome this, we use equivalent operator preconditioning, similarly as in [Kir10]. However, just as for other such methods, the standard convergence estimates become arbitrarily slow if $\varepsilon \to 0$, namely, the constants in the convergence estimate blow up as $\varepsilon \to 0$.

Our goal is to prove that the convergence using streamline diffusion preconditioning can in fact be robust, i.e. to give bounds independently of ε for proper convection vector fields. We prove this via an improved "streamline" Poincaré–Friedrichs inequality. Altogether, our aim is to show that a suitable combination of the two approaches (streamline diffusion finite elements and equivalent operator preconditioning) results in a robust extension of the latter to certain convection-dominated problems, namely the constants are not deteriorating. Our theoretical results are illustrated using various numerical experiments.

The convection-dominated problem

For simplicity we present the results in detail for a simple class of problems with Dirichlet boundary conditions:

$$\begin{cases} -\varepsilon\Delta u + \boldsymbol{w} \cdot \nabla u = g \qquad \text{in } \Omega \\ \qquad\qquad u|_{\partial\Omega} = 0. \end{cases}$$

We assume that $\Omega \subset \mathbb{R}^d$ is a polyhedral domain. The convective vector field $\boldsymbol{w} \in C^1(\overline{\Omega}, \mathbb{R}^n)$ satisfies $\operatorname{div} \boldsymbol{w} = 0$, and $g \in L^2(\Omega)$. For more complicated problems we refer to [AKK14].

The weak equation,

$$a(u,v) := \int_\Omega \big(\varepsilon\, \nabla u \cdot \nabla v + (\boldsymbol{w} \cdot \nabla u)v\big) = \int_\Omega gv \qquad (v \in H_0^1(\Omega)),$$

will be stabilized using an extra term.

The streamline diffusion finite element method and preconditioning

Let $\mathcal{T}_h = \{T_k\}_{k=1}^K$ be a triangulation of Ω, and $V_h \subset H_0^1(\Omega)$ be the corresponding subspace of continuous, piecewise linear basis functions, then we set

$$\int_\Omega \left(\varepsilon \nabla u_h \cdot \nabla v_h + (\boldsymbol{w} \cdot \nabla u_h) v_h\right) + \sum_{k=1}^K \delta_k \int_{T_k} (\boldsymbol{w} \cdot \nabla u_h)\,(\boldsymbol{w} \cdot \nabla v_h) = \int_\Omega g(v_h + \delta \boldsymbol{w} \cdot \nabla v_h) \tag{3}$$

$\forall v_h \in V_h$, where $\delta_k > 0$ is a set of elementwise constant parameters. This approach is the streamline diffusion finite element method (SDFEM), cf. [ESW14, Chapter 3].

The left-hand side of (3) is called the streamline diffusion bilinear form, denoted by a_{SD}, together with the corresponding streamline diffusion inner product $\langle .,. \rangle_{SD}$, being the symmetric part of it, with the induced norm $\|.\|_{SD}^2$.

The streamline diffusion method involves proper choice of the parameters δ_k. For a fixed convection field and uniform parameters on a regular mesh a widespread choice is $\delta = O(h)$. Then the SDFEM converges as $\|u - u_h\|_{SD} = O(h^{3/2})$, cf. [ESW14, Chapter 3]. It is important to note that the parameters δ_k are chosen independently of ε.

The discrete problem $\boldsymbol{A}\boldsymbol{c} = \boldsymbol{b}$ is preconditioned with the stiffness matrix $\boldsymbol{S}$ corresponding to the inner product $\langle .,. \rangle_{SD}$, serving as a preconditioner to the discrete system:

$$\boldsymbol{S}^{-1}\boldsymbol{A}\boldsymbol{c} = \tilde{\boldsymbol{b}} = \boldsymbol{S}^{-1}\boldsymbol{b}. \tag{4}$$

The preconditioning matrix $\boldsymbol{S}$ is called *streamline diffusion preconditioner.* We note that, in simple cases, $\boldsymbol{S}$ is the symmetric part of $\boldsymbol{A}$. The main idea of equivalent preconditioning in the context of bilinear forms is that the bounds are inherited uniformly by the stiffness matrices as: If the form a_{SD} has the bounds

$$|a_{SD}(u_h, v_h)| \le M\|u_h\|_{SD}\|v_h\|_{SD}, \qquad a_{SD}(u_h, u_h) \ \ge m\|u_h\|_{SD}^2 \qquad (\forall u_h,\, v_h \in V_h),$$

then $\boldsymbol{S}^{-1}\boldsymbol{A}$ inherits the same bounds w.r.t. the $\boldsymbol{S}$-norm, i.e.

$$|\langle \boldsymbol{S}^{-1}\boldsymbol{A}\boldsymbol{c},\, \boldsymbol{d}\rangle_{\boldsymbol{S}}| \le M\,|\boldsymbol{c}|_{\boldsymbol{S}}\,|\boldsymbol{d}|_{\boldsymbol{S}}, \qquad \langle \boldsymbol{S}^{-1}\boldsymbol{A}\boldsymbol{c},\, \boldsymbol{c}\rangle_{\boldsymbol{S}} \ge m\,|\boldsymbol{c}|_{\boldsymbol{S}}^2 \qquad (\forall\, \boldsymbol{c}, \boldsymbol{d} \in \mathbb{R}^d).$$

In the results of Kirby [Kir10], using the standard Poincaré–Friedrichs inequality, only the ε dependent bound

$$M \le 1 + \frac{C_\Omega}{\sqrt{\delta_0 \varepsilon}}$$

can be shown, which, for small values of ε, is extremely huge, therefore it yields an increasing number of required iterations as ε approaches zero. It is easy to see that the lower bound is $m = 1$.

Robust convergence results

Showing a robust upper bound M the key result is the following.

Theorem 3.1 (Streamline Poincaré–Friedrichs inequality [AKK14])**.** *Let $\boldsymbol{w} \in C^1(\overline{\Omega}, \mathbb{R}^d)$, for which $\boldsymbol{w}(\boldsymbol{x}) \neq 0$ ($\boldsymbol{x} \in \Omega$), be a globally rectifiable vector field on $\overline{\Omega}$.*

Then there exists a constant $C_{\boldsymbol{w}} > 0$, depending on $\boldsymbol{w}$ but independent of v such that

$$\|v\|_{L^2(\Omega)} \le \ C_{\boldsymbol{w}}\, \|\boldsymbol{w} \cdot \nabla v\|_{L^2(\Omega)} \qquad (v \in H_0^1(\Omega)).$$

The restrictive conditions $\boldsymbol{w}(\boldsymbol{x}) \neq 0$ and the global rectifiability can be weakened, see [AKK14].

Using this result the following convergence estimates can be shown.

Theorem 3.2 ([AKK14])**.** *Let $\boldsymbol{w} \in C^1(\overline{\Omega}, \mathbb{R}^d)$, for which $\boldsymbol{w}(\boldsymbol{x}) \neq 0$ ($\boldsymbol{x} \in \Omega$), be a globally rectifiable vector field on $\overline{\Omega}$. Then the linear convergence of the conjugate gradient method for the preconditioned system* (4) *is bounded independently of ε. Namely, for the GCG-LS method, the residual satisfies*

$$\left(\frac{\|r_k\|}{\|r_0\|}\right)^{1/k} \leq \left(1 - \frac{1}{M^2}\right)^{1/2} = \frac{\sqrt{C_{\boldsymbol{w}}(C_{\boldsymbol{w}} + 2\delta_0)}}{C_{\boldsymbol{w}} + \delta_0} \qquad (k = 1, 2, \ldots, N),$$

and for the CGN method

$$\left(\frac{\|r_k\|}{\|r_0\|}\right)^{1/k} \leq 2^{1/k}\frac{M-1}{M+1} = 2^{1/k}\frac{C_{\boldsymbol{w}}}{C_{\boldsymbol{w}} + 2\delta_0} \qquad (k = 1, 2, \ldots, N),$$

where both estimates are independent of ε.

Numerical tests, with a simple and an enclosed flow, are reinforcing our theoretical results. We show the iteration numbers and CPU times with PCGN on the disc with flow $(-y, x)$, and the iteration numbers together with the old and new bounds.

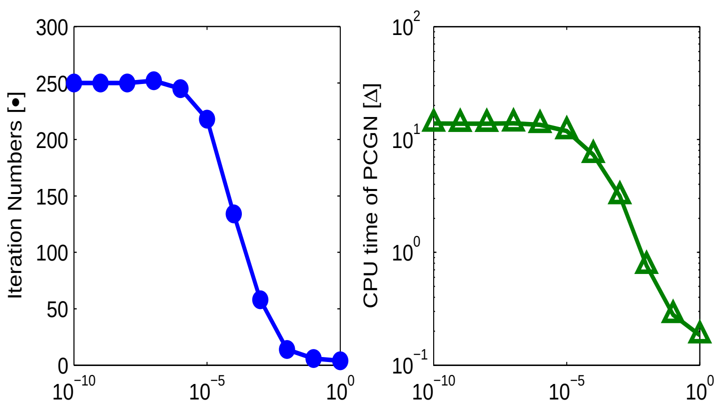

Figure 1: Iteration numbers and CPU times with PCGN

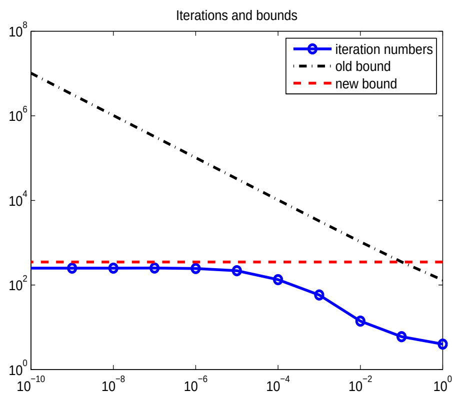

Figure 2: Iteration numbers vs the old and new bounds

4. A comparison of some efficient numerical methods for nonlinear elliptic problems

In [Kov12] computational efficiency of three iterative methods is studied: namely, the *gradient method*, the *Newton method* and the *quasi-Newton method*, using a semilinear elliptic model problem of heat transfer. It is shown that each of the methods can be the fastest regarding CPU time for certain parameters, although, as expected, this case is exceptional for the gradient method. A suitable version of quasi-Newton method is proposed and shown to be the least costly in most cases. Based on our first experiences we propose some improvements for the iterative methods, having a serious practical value.

Let us consider the model problem :

$$\begin{cases} -\operatorname{div}\big(k(x)\nabla u\big) + \sigma(x)|u|^3 u = g(x) & \text{in } \Omega \\ k(x)\partial_\nu u + \alpha(x)\big(u - \tilde{u}(x)\big) = 0 & \text{on } \partial\Omega, \end{cases} \tag{5}$$

The three investigated iterative methods applied to the model problem are the following: the gradient method, Newton's method, and a quasi-Newton method (where the reaction term is approximated with a constant). For their convergence results we refer to [FK02] or [Kov12]. In particular for the quasi-Newton method the following theorem holds:

Theorem 4.1. *Let F denote the weak operator corresponding to (5), and let B_n be the approximation of $F'(u_n)$. Then there exist bounds $M_n \geq m_n > 0$ such that*

$$m_n \langle B_n v, v\rangle \leq \langle F'(u_n)v, v\rangle \leq M_n \langle B_n v, v\rangle \qquad (v \in H^1(\Omega), n \in \mathbb{N}), \tag{6}$$

where $M_n = 2$, $m_n = \big(1 + \tilde{c}_n D d^{-1} \max\{D, {\alpha_{\inf}}^{-1}\}\big)^{-1}$ for all $n \in \mathbb{N}$, $D = \operatorname{diam}(\Omega)$ where $\Omega \subset \mathbb{R}^d$, $\tilde{c}_n = 2\max\big\{\sigma|u_n|^3\big\}$ and $\alpha_{\inf} := \inf_\Omega \alpha$.

Corollary 4.1 ([Kov12]). *Using the above bounds, we have the following convergence result:*

$$\limsup \frac{\|F(u_{n+1})\|}{\|F(u_n)\|} \leq 1 - \frac{2}{3 + 2Dd^{-1}\limsup\Big(\tilde{c}_n \max\{d, {\alpha_{\inf}}^{-1}\}\Big)}\ .$$

Based on our numerical experiments the theoretically given convergence orders can be seen: gradient method is linear, the quasi-Newton method is superlinear, and Newton's method is quadratic, in both one and two dimensions. Mesh independence is numerically observed.

There occurred very little CPU time difference between quasi-Newton and Newton method, however, both easily outperformed the usual gradient method. Taking into account the difficulties of implementations, the computational costs, and considering the little time difference, we advise to use quasi-Newton method with a piecewise constant preconditioner. Even with a low number of subdomains it easily overcomes Newton's method. On the other hand, practically, we cannot completely reject either of these methods.

Based on the results presented here, from now on, the thesis will focus on *variable preconditioning quasi-Newton method* and *Newton method* (usually *with an inner CG iteration*).

5. Sharp a posteriori error estimation for nonlinear elliptic problems

A common and important issue in numerics is the error estimation of the numerical methods. In [Kov14] we aim to discuss a *sharp upper global a posteriori error estimator* developed in [KK09].

We check the numerical performance, demonstrate the efficiency and accuracy of this estimator using a second order elliptic quasilinear equation. The focus is on the technical and numerical aspects and on the components of the error estimation, especially on the adequate solution of the involved auxiliary problem, which enables *sharpness* in the sense that by the investment of "computation time" the true error can be estimated by any desired precision.

We consider an abstract problem $F(u)+l=0$, and a model problem:

$$\begin{cases} -\operatorname{div}\Big(a\big(|\nabla u|^2\big)\nabla u\Big) = g & \text{in } \Omega \\ u|_{\partial\Omega} = 0, \end{cases} \tag{7}$$

having a unique weak solution according to [FK02, Theorem 6.4].

The error is measured using the energy type error functional:

$$E(u) = \langle F(u) - F(u^*), u - u^* \rangle.$$

Adapting [KK09, Theorem 3.1] the following estimate holds for quasilinear problems: Let $u_h \in W^{1,\infty}(\Omega)$ an approximate weak solution of (7). Then for arbitrary $z \in L^\infty(\Omega)^d$ such that $z \in H(\operatorname{div},\Omega)$ and arbitrary $w \in H_0^1(\Omega)$,

$$\begin{aligned} E(u_h) \le\ \operatorname{EST}\big(u_h; z, w\big) := \Big(& m^{-1/2}\, c_\Omega \,\|\operatorname{div} f(z) + b\|_{L^2(\Omega)} + \frac{L}{2}\, m^{-3/2}\, D(u_h; z, w) \\ &+ \Big(\langle f(\nabla u_h) - f(z), \nabla u_h - z\rangle_{L^2(\Omega)^d} + \frac{L}{2m}\, D(u_h; z, w)\, \|\nabla u_h - z\|_{L^2(\Omega)^d}\Big)^{1/2}\Big)^2, \\ \text{where}\quad D(u_h; z, w) := \Big(& M\|z - \nabla w\|_{L^2(\Omega)^d} + c_\Omega \|\operatorname{div} f(z) + b\|_{L^2(\Omega)}\Big)\|\nabla u_h - z\|_{L^\infty(\Omega)^d}, \end{aligned}$$

where $M \ge m > 0$ are the spectral bounds of $F'(u)$, and L is its Lipschitz constant, finally $c_\Omega > 0$ is the constant appearing in the Poincaré–Friedrichs inequality.

We solve the weak nonlinear problem with a Newton-like method. Then it is important to determine good candidates for z^* and w^* in $\operatorname{EST}\big(u_h; z^*, w^*\big)$: For the parameter z^* should be a sufficiently accurate approximation of the gradient of u^*, by the suggestions made in [KK09], we use some *averaging operator* G_h to set $z^* = G_h(\nabla u_h)$, having a better approximation:

$$\|\nabla u^* - G_h(\nabla u_h)\| \le ch^2, \qquad \text{instead of} \qquad \|\nabla u^* - \nabla u_h\| \le ch.$$

Finally, the last missing parameter w^* is defined as the weak solution of the linear *auxiliary problem*:

$$\begin{cases} -\Delta w = -\operatorname{div} z^* & \text{in } \Omega \\ w|_{\partial\Omega} = 0. \end{cases}$$

The constants of the estimator are given by the following result.

Proposition 5.1 ([Kov14]). *The following statements are true for the weak operator F, corresponding to a problem modeling elasto-plastic tension, with the nonlinearity $a(\eta) = \min\Big\{\frac{1.02}{1+\sqrt{1-\frac{\eta}{3}}}, a(\eta_0)\Big\}$, with $\eta_0 = 2.6$.*

(i) There exist constants $M \ge m > 0$, independent of u and p such that the derivative of F satisfies

$$m\|p\|^2 \le \langle F'(u)p, p\rangle \le M\|p\|^2,$$

$$\text{where} \qquad m = a(0) = 0.51 \qquad \text{and} \qquad M = a(\eta_0) + 2a'(\eta_0)\eta_0 \approx 2.046213.$$

(ii) The derivative, $F' : W^{1,\infty}(\Omega) \to B(H_0^1(\Omega))$, is also Lipschitz continuous with constant $L \approx 11.935094$.

(iii) Finally the Poincaré–Friedrichs constant is $c_\Omega = \dfrac{2}{\pi}$.

Our experiments in [Kov14] show that this estimator cooperates well with different nonlinear iterative solvers. It is also illustrated that the estimator is indeed efficient and sharp, and highly applicable for a posteriori error estimation. It only requires just a few parameters to compute.

The sharpness of the estimation is in a close connection with the accuracy of the numerical solution of the linear auxiliary problem. To be precise: both in EST and in D the dominant terms are multiplied by a term, that can be decreased by a better solution of the auxiliary problem.

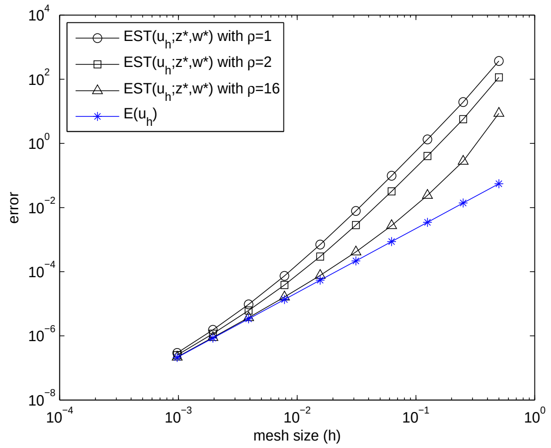

Figure 3: Log-log plot of errors and estimated errors, with ρ-refined meshes (one dimension)

$h = 1/2^k$	$E(u_h)$	$\mathrm{EST}(u_h; z^*, w^*)$	EST $/E$
1	0.055037791	371.914078575	6757.43
2	0.013856122	19.345738838	1396.18
3	0.003470203	1.329380121	383.08
4	0.000867929	0.098033794	112.95
5	0.000217006	0.007817070	36.02
6	0.000054252	0.000699770	12.89
7	0.000013563	0.000073833	5.44
8	0.000003390	0.000009569	2.82
9	0.000000847	0.000001531	1.80
10	0.000000211	0.000000291	1.37

Table 1: Comparison of error and estimated error for the original mesh (one dimension)

6. Variable preconditioning in complex Hilbert spaces

In this chapter we develop a damped Newton-like method, with a stepwise variable preconditioner, for solving complex nonlinear operator equations. This is a nontrivial complex Hilbert space extension of a preconditioning iterative method developed by Karátson and Faragó in [KF03] for real Hilbert spaces.

The motivation for this extension comes from the fully discrete numerical solution of the time-dependent nonlinear Schrödinger equation. We use the *Rothe-method* [Rot30] for the numerical solution of the (complex) nonlinear Schrödinger equation: first applying a time discretization, then use our method to obtain the solution of the complex nonlinear elliptic boundary value problems on each time level.

We show global convergence up to second order via a damped preconditioned iterative method, where the preconditioner is obtained by spectral equivalence. The result is provided by a number of preliminary lemmas and it follows the classical ideas of the usual convergence proofs for damped quasi-Newton methods.

First we formulate this well-known equation of quantum mechanics, the nonlinear Schrödinger equation:

$$\begin{cases} \dfrac{1}{\mathrm{i}}\partial_t u - \Delta u + k|u|^2 u = g, & \text{in } \Omega \times [0,T) \\ \qquad\qquad u|_{\partial\Omega} = 0 \end{cases}$$

where $u : \Omega \to \mathbf{C}$ is the unknown function and k is some positive real constant. The letter i denotes the imaginary unit.

Applying Rothe's method, using the backward Euler method, we obtain the following nonlinear elliptic equation in each time step:

$$\frac{1}{\mathrm{i}\tau}u^{j+1} - \Delta u^{j+1} + k|u^{j+1}|^2 u^{j+1} = \frac{1}{\mathrm{i}\tau}u^j + g^{j+1},$$

whose weak formulation defines the nonlinear operator equation $\langle F(u^{j+1}), v\rangle = 0 \quad (v \in H)$ with a complex Hilbert space H.

A damped quasi-Newton method as variable preconditioning in a complex Hilbert space

We develop a damped quasi-Newton method with a stepwise variable preconditioner. The original result of [KF03] were proved by self-adjoint theory, which cannot be applied in the complex framework, therefore our proofs are more direct.

We consider an operator equation

$$F(u) = 0,$$

solved by the iterative method described in the following theorem.

Theorem 6.1 ([KK13]). *Let $\big(H, \langle ., .\rangle\big)$ be a complex Hilbert space, with induced norm $\|.\|$. Let the operator $F : H \to H$ have a symmetric, coercive and bounded Gâteaux derivative, which is also Lipschitz continuous and the F satisfies the conditions below.*

Let $u^* \in H$ denote the unique solution of equation $F(u) = 0$. Starting from arbitrary $u_0 \in H$, let us define the approximating sequence $(u_n) \subset H$ by

$$u_{n+1} := u_n - \eta_n G_n^{-1} F(u_n) \qquad (n \in \mathbb{N}),$$

with the damping parameter η_n. The following conditions are also satisfied:

(iii) If u_n is constructed then we choose a self-adjoint operator $S_n \in B(H)$ spectrally equivalent to $\operatorname{Re} F'(u_n)$:

$$m_n \langle S_n v, v\rangle \le \operatorname{Re}\langle F'(u_n)v, v\rangle \le M_n \langle S_n v, v\rangle \qquad (v \in H, n \in \mathbb{N})$$

holds with some constants $M_n \ge m_n > 0$, and assume that there exist constants $K > 1$ and $\varepsilon > 0$ such that $M_n/m_n \le 1 + 2/\big(\varepsilon + K\mu(u_n)\big)$, where $\mu(u_n) := L\Lambda^2\lambda^{-4}\|F(u_n)\|$. Further, we let $G_n \in B(H)$ such that

$$\operatorname{Re} G_n = \frac{M_n + m_n}{2} S_n \qquad \text{and} \qquad \operatorname{Im} G_n = \operatorname{Im} F'(u_n).$$

(iv) Let the operators G_n satisfy $\|(\operatorname{Re} G_n)v\|_n \le \|G_n v\|_n$ ($v \in H$, $n \in \mathbb{N}$), where $\|v\|_n^2 = \operatorname{Re}\langle F'(u_n)^{-1}v, v\rangle$.

(v) We define the damping parameter as $\eta_n = \min\left\{1, \frac{1-Q_n}{2\varrho_n}\right\}$, where $\mu(u_n)$ is the same as in condition (iii) and

$$Q_n = \big(1 + \mu(u_n)\big)\frac{M_n - m_n}{M_n + m_n}, \qquad \varrho_n = \frac{2L\Lambda^{3/2}M_n^2}{\lambda^{7/2}(M_n + m_n)^2}\|F(u_n)\|$$

The damping parameter η_n ensures an optimal contractivity in the n^{th} step in the $\|.\|_*$-norm.

Then the following convergence result holds. We have

$$\|u_n - u^*\| \le \lambda^{-1}\|F(u_n)\| \to 0,$$

namely, using the norm $\|v\|_*^2 = \mathrm{Re}\langle F'(u^*)^{-1}v, v\rangle$*:*

$$\limsup \frac{\|F(u_{n+1})\|_*}{\|F(u_n)\|_*} \le \limsup \frac{M_n - m_n}{M_n + m_n} < 1.$$

Moreover, if in addition $M_n/m_n \le 1 + c_1\|F(u_n)\|^\gamma \quad (n \in \mathbb{N})$ *is satisfied with some constants* $c_1 > 0$ *and* $0 < \gamma \le 1$*, then* $\|F(u_{n+1})\|_* \le d_1\|F(u_n)\|_*^{1+\gamma}$*, hold with some* $d_1 > 0$*.*

The conditions of the above theorem can be relaxed. It suffices to assume the boundedness and Lipschitz continuity only locally:

Proposition 6.1 ([KK13])**.** *Let the conditions of Theorem 6.1 hold, but we only assume local boundedness and local Lipschitz continuity:*

$$|\langle F'(u)v, w\rangle| \le \Lambda(\|u\|)\,\|v\|\,\|w\| \qquad \text{and} \qquad \|F'(u) - F'(v)\| \le L(\max\{\|u\|, \|v\|\})\,\|u - v\|$$

for suitable nondecreasing functions $\Lambda, L : \mathbb{R}^+ \to \mathbb{R}^+$*. Then the analogous convergence result holds.*

The following theorem shows, that our method is applicable for the time discretization of the nonlinear Schrödinger equation.

Theorem 6.2 ([KK13])**.** *Let* F *be the elliptic operator obtained after time discretization, let* $G_n := \frac{M_n+m_n}{2}S_n + \mathrm{i}\,\mathrm{Im}\,F'(u_n)$ *be the approximation of* $F'(u_n)$*. Then all the properties of Proposition 6.1 hold, with* $M_n \ge m_n > 0$ *given as*

$$m_n = \frac{1}{1 + K_{2,\Omega}^2 \max \omega_n}, \qquad M_n = 1 + 3kK_{4,\Omega}^4\|u_n\|^2\,.$$

7. A general numerical code

As the number of different problems, which we were able to numerically handle here, reached a certain barrier, it has naturally arisen to combine their codes into a unified framework. The aim is to solve a very general parabolic partial differential equation, or a system of such equations, using the codes accumulated over the years. Here this nontrivial "byproduct" is described.

Let us consider a *semilinear parabolic* problem on the domain $\Omega \subset \mathbb{R}^2$, with boundary $\partial\Omega = \Gamma_D \cup \Gamma_N$:

$$\begin{cases} \partial_t u - \mathrm{div}\Big(k(x,t)\nabla u\Big) + \boldsymbol{w}(x,t)\cdot\nabla u + q(x,t,u) = g(x,t) & (x \in \Omega,\ t \in (0,T)), \\ u(x,t) = u_0(x,t) & (x \in \Gamma_D,\ t \in (0,T)), \\ \partial_{\nu_{k(x,t)}} u + s(x,t,u) = \gamma(x,t) & (x \in \Gamma_N,\ t \in (0,T)), \\ u(x,0) = u_0(x,0) & (x \in \Omega). \end{cases}$$

In addition *systems of* r *equations* of the same structure can be handled, naturally, coupled in the semilinear term, and in the Neumann-boundary through s. Furthermore, the code is able to solve problems with *interface* conditions over a curve Γ, of a similar style as the Neumann-type boundary conditions.

A main objective of the package is to solve the problems in a user friendly way, in other words the code functions as a black box tool.

Discretizations and the used numerical methods

We use the Rothe approach coupled with the finite element method. The resulting weak nonlinear elliptic problem is solved by an inner–outer iteration. The outer iteration is the *damped inexact Newton method*, the arising linear auxiliary problems are solved with a *preconditioned conjugate gradient method*, cf. [Axe96, FK02]. As a preconditioning operator we use the linear principal part, cf. [FK02, Section 8.2.4], which enables to decouple the linear system into r smaller problems. We use Lagrangian finite elements for the spatial discretization, therefore the reference element based assembly techniques are implemented.

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